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# Verification Procedures Applied to the U.S. EPA (Environmental Protection Agency) Regional Oxidant Model

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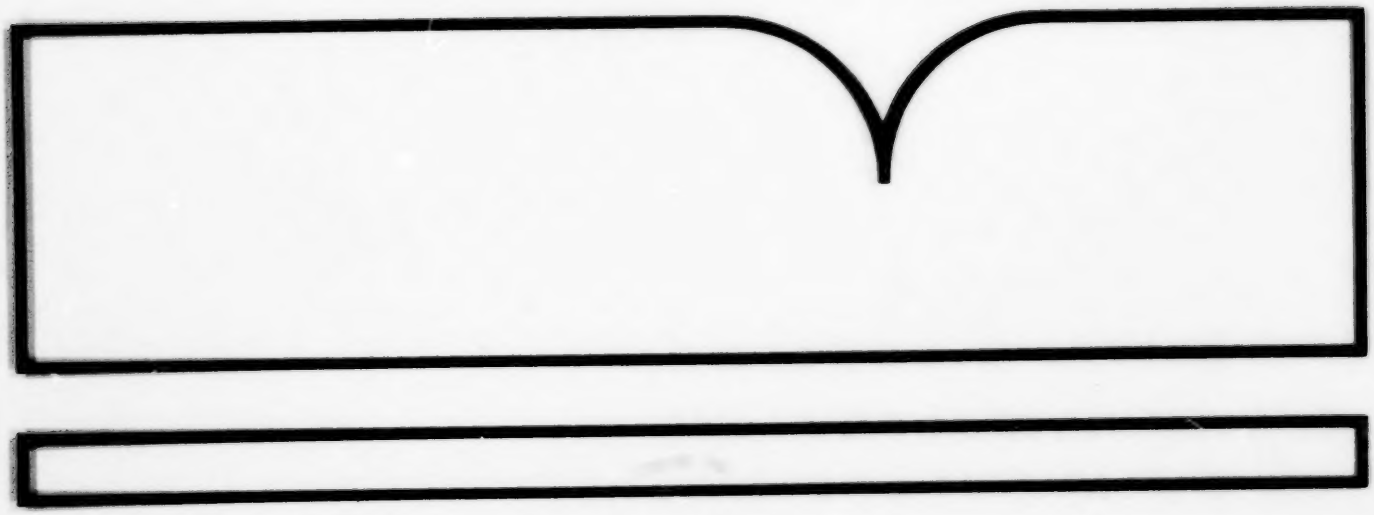

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# VERIFICATION PROCEDURES APPLIED TO THE U.S. EPA REGIONAL OXIDANT MODEL

by

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Regional air quality simulation models have been developed as research tools to gain a greater understanding of long range transport and transformation of air pollutants and to evaluate regional control strategy alternatives. To ensure credibility of these complex model predictions, the performance of model codes must be verified for their adherence to theoretical formulations, accuracy of numerical algorithms, ability to reproduce observed data and sensitivity to uncertainties in input data.

This paper describes the procedures used for verification of the U.S. EPA Regional Oxidant Model. Comparisons with observed data are presented together with a brief summary of the results from two ozone control strategy applications. The sensitivity of the model to known uncertainties in input data is discussed in relation to its effect on air pollution control strategy evaluation.

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## INTRODUCTION

Over the past several years the U.S. Environmental Protection Agency (EPA) has been developing and testing a photochemical model capable of simulating regional transport and transformation of ozone and its precursors. Specific applications of this Regional Oxidant Model (ROM) are intended to evaluate the effectiveness of emission control strategies. Regulatory decisions on emissions control may, in part, be influenced by economic analyses which are based on model air quality predictions. Thus the reliability of these model predictions are of utmost importance to the policy analysts, especially in the absence of alternate forecasts of ozone spatial distribution and maxima. The purpose of this paper is to discuss the variety of verification procedures applied to ROM to ensure the reliability of the model predictions and appropriate interpretation of these model results.

## OVERVIEW OF THE REGIONAL OXIDANT MODEL

The ROM is an Eulerian model with horizontal resolution of approximately 18.5 km over spatial domains up to 1000 km. It has three layers in the vertical which dynamically vary in space and time in response to local physical processes. The model also uses a shallow diagnostic surface layer to parameterize subgrid scale effects and surface deposition. ROM is designed to simulate all of the important physical and chemical processes thought to affect the production and transport of ozone on a regional scale (1000 km). These processes include horizontal transport, atmospheric chemistry, turbulence and wind shear effects, cumulus cloud effects, mesoscale vertical motion and eddy effects, terrain effects on horizontal flows and on deposition and diffusion, emissions of natural and man-made precursors, and wet and dry removal processes. A detailed description of the theoretical basis of ROM is presented elsewhere (Lamb, 1983).

The theoretical basis, however, is only one aspect of a model's credibility. The implementation of that theory and the reliability of the required input data also warrant careful consideration. As shown in Figure 1,

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ROM has been implemented in a general modeling framework that can readily incorporate the latest advances in atmospheric science. The core of the system is a set of algorithms which solve the coupled set of generalized finite difference equations that describe the governing processes in each layer of the model. These governing equations have been expressed in a form which allows the chemical kinetics, advection, and vertical flux to be treated independently. All physical and chemical parameters such as wind components, vertical velocity and diffusivity fields, chemical rate constants and source emissions, etc. are input into the model core in the form of complex matrix coefficients. These coefficients can no longer be equated with physical reality; they are purely mathematical entities related specifically to the form of the generalized finite difference algorithms. These matrix inputs are computed in a B-Matrix Compiler (BMC) which draws upon over fifty Model Input Files for the data necessary to compute the matrix coefficients. The parameters in the Model Input Files are the output from a series of approximately thirty programs which process observed meteorology, land use and topography data, and estimated precursor emissions. Many of these processors are complex models themselves. For example, one processor generates families of vertically integrated horizontal winds for each model layer which are consistent in space and time with observed meteorology and physical principles, while another processor refines the nighttime winds by solving the shallow water equation. All processors are interconnected in a hierarchical fashion by their requirements for and production of data. A complete description of the ROM input processor network design has been published (Lamb, 1984).

## ROM VERIFICATION PROCESS

The modular design of the ROM not only provides flexibility for incorporating scientific updates, but also provides an organizational framework for implementing verification procedures. The magnitude and complexity of ROM as well as the regulatory nature of its application demand stringent and formal quality control encompassing all aspects - initial design through final interpretation. The quality assurance program for ROM consists of four major phases which extend over the entire lifetime of the system: software development, data verification, model evaluation, and model applications.

### Software Development

The Jackson Structured Programming method (Jackson, 1975) has been used in the implementation of ROM from its inception. Thus coding conventions, documentation, and data exchange are fairly uniform throughout the system even though a team of programmers was responsible for the implementation and enhancement over a period of several years. Each major module is coded according to published specification documents (Lamb, 1983, 1984) and tested individually to verify performance through an expected range of input values. Out-of-range input values produce warning messages. Processor testing includes hand calculations when possible, review of minimum/maximum values, and review of graphical presentation of data for each hour of a complete 24 hour period. The predictions of individual components are also compared against measured data whenever possible. For example, the vertical cloud flux is compared with ambient aircraft measurements and the chemical kinetics mechanism is evaluated against smog chamber data. Auxiliary processors required to handle special functions such as reformatting or interpolating data are treated similarly; however, specifications are only informally documented. Efforts are underway to complete formal documentation of the entire system. The final code is compared to the written specifications and necessary adjustments in code or documentation are made to ensure consistency.

# OVERVIEW OF REGIONAL OXIDANT MODELING SYSTEM

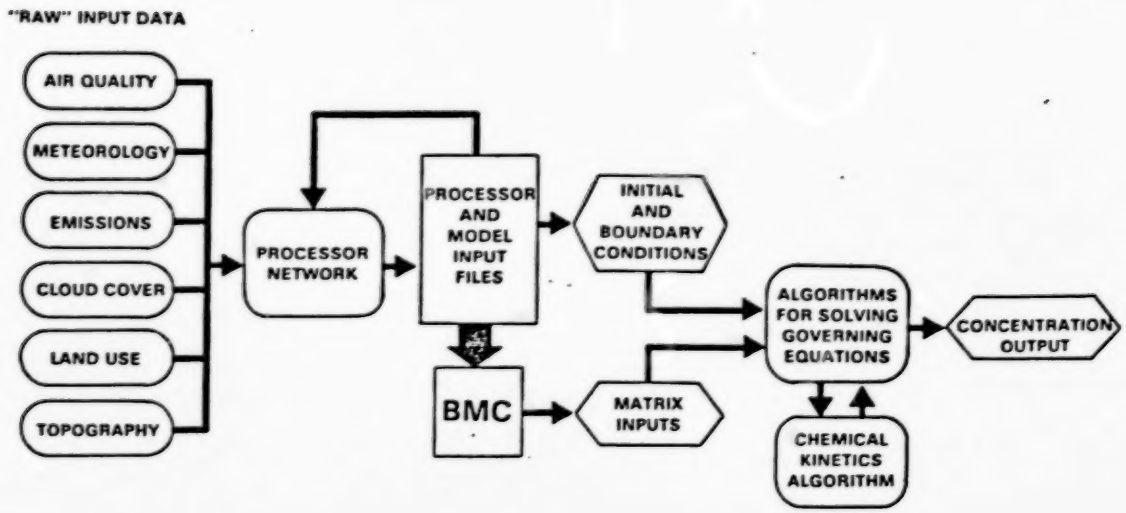


Figure 1. Overview of Regional Oxidant Modeling System.

If the code is modified another testing cycle is required. The code is then moved to a write-protected software library where version identification and internal software audit features are added, and a final representative benchmark is executed and saved. At this point the module becomes part of the controlled production software library. At various stages in the processor network development groups of processors and finally the entire processor system are executed to ensure appropriate system-wide interaction and function.

The core model itself requires additional testing to ensure the accuracy of numerical predictions and to demonstrate the fundamental capability of the model to simulate multiday plume transport and the effects of plume interaction. The differential equations that describe the governing chemical and physical processes cannot be solved analytically, therefore they are implemented in computer code by numerical algorithms which closely approximate a true differential solution. The performance of these algorithms is difficult to evaluate for real environmental conditions because an exact solution is unknown, but they can be tested by applying the model to simple hypothetical problems with known exact solutions.

A series of tests were performed on the first generation ROM to assess the performance of the chemical kinetics algorithm independently and in combination with the other major algorithms -- transport/diffusion and vertical fluxes (Lamb and Laniak, 1985). One particular experiment which placed four continuous line sources of hydrocarbon and $NO_x$ in a circular wind field was able to quantify the effects of truncation error, the rate of error growth over multiday simulations, the compounding effects of interacting plumes, error levels at domain boundaries, and the error caused by positively resetting negative concentrations in the transport algorithm. A similar series of tests are currently being performed on the second generation ROM to evaluate how accurately the algorithms represent the motion and slopes of the layer surfaces. The major differences between the first and second generation ROM are listed below:

| | First Generation | Second Generation |
|---|---|---|
| Layer Thickness: | Constant | Variable in space & time |
| Winds: | Nondivergent | Divergent |
| Chemistry: | Demerjian-Schere | Carbon Bond IV |
| Emissions: | Anthropogenic | Anthropogenic plus Biogenic hydrocarbon |

Results of these tests provide a necessary condition for model validity -- quantification of the accuracy of the numerical algorithms. However, the planned application of ROM in support of regulatory decision making requires a more thorough and formal evaluation of the final model predictions. Prerequisite to model execution for this evaluation is the verification of raw and processed model input data.

## Input Data Verification

Of the six types of raw input data required by ROM, shown in Figure 1, the meteorological data and emissions require the most quality control. The quality of the other data sets, however, cannot be ignored and do receive an appropriate level verification. Ambient ozone measurements used for model boundary conditions are screened for outliers, local plume effects, and representativeness for background conditions. Cloud cover, land use, and topography data are compared with available maps. All upper air and hourly surface meteorological data are processed by standard

quality control programs which perform range checks, limit checks, and flag unrealistic physical relationships. Any suspect data are manually reviewed and eliminated if shown to be unreasonable.

The anthropogenic emissions data currently used in ROM are provided by the National Acid Precipitation Assessment Program's (NAPAP) Task Group on Emissions and Controls. The basic information for estimating annual emissions are taken from EPA's National Emissions Data System (NEDS). Primarily the data consist of statistically averaged emission factors and fuel consumption estimates which are used to calculate annual emissions of the five criteria pollutants: TSP, $SO_x$, $NO_x$, VOC, CO. Point source emissions estimates are based on individual source or process data whereas area source emissions are based on county level fuel consumption or activity estimates. ROM primarily uses emissions in hourly gridded form thus requiring additional assumptions to be made in apportioning emissions to the required spatial, temporal, and species resolution. Thus a knowledge of the accuracy of the gridded hourly emissions is essential for confident interpretation of the model results for regulatory support.

A review of anthropogenic emissions inventory development efforts during the past few years provides a startling awareness of the impact of emissions inventory updates on successive gridded emissions estimates for the same base year - 1980. These updates include improvements in methodologies for calculation of emissions, error correction, and the incorporation of more recent data such as 1980 vs 1970 census data and revised AP-42 emission factors. The Northeast Corridor Regional Modeling Project (NECRMP) was one of the earliest attempts to provide detailed ozone precursor (VOC, $NO_x$) emissions required by regional models using nonlinear chemistry mechanisms. Figure 2 compares 200 grid cells with highest emissions (point and area source combined) of nitrogen oxides in the Northeastern U.S. The regression line indicates that the NAPAP 4.2 inventory updates have reduced the estimated emissions of grids that were strongest in NECRMP and elevated the estimated emissions of the weaker grids. These differences may be attributed to spatial shifts due to the use of updated census data for spatial allocation or to improved mobile emissions factors. Figure 3 compares two successive versions of the NAPAP NO inventory. The bulk of the data show high correlation; no bias appears, but the magnitude of the outliers again raises a question of how close even these improved estimates are to the actual emissions from the domain. The variability in successive estimates of gridded 1980 base year emissions is over 10 times larger than the changes that control strategy implementation would cause. In ROM the predicted response of ozone concentrations to emission reductions is a function of the base emission levels. If base emissions contain large uncertainties, the usefulness of the model predictions, especially for regulatory support, may be of questionable value. This issue of the accuracy of emission estimates and the sensitivity of model predictions to emissions variability is a prime focus in current research planning.

The Carbon Bond IV chemical kinetics mechanism in the second generation ROM incorporates specific chemical reactions for isoprene, a hydrocarbon species naturally emitted from vegetation. Three basic components are necessary to estimate hourly gridded biogenic hydrocarbons compatible with ROM: 1) emission factors representative of vegetative species indigenous to the modeling region, 2) empirical relationships between emission factors and specific environmental parameters such as temperature and solar intensity which may influence those factors, and 3) quantitative estimates of vegetation density of the representative species in a designated area. Details of the inventory used in ROM are given by Novak and Reagan (1986). Large uncertainties are associated with emission factors and much more work is needed in this area. However, current hydrocarbon

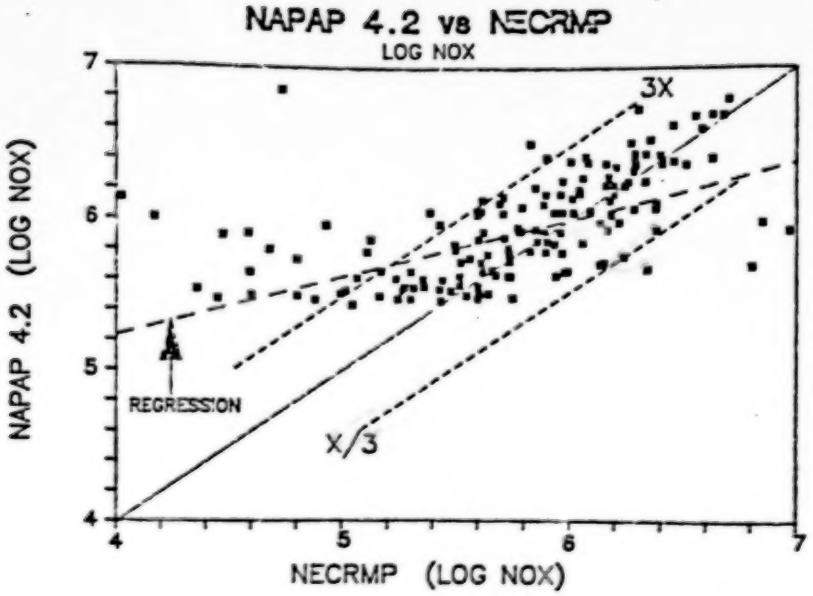


Figure 2. Comparison of NAPAP 4.2 and NECRMP gridded VOC emissions for the 200 strongest source cells in the Northeastern U.S. ROM domain.

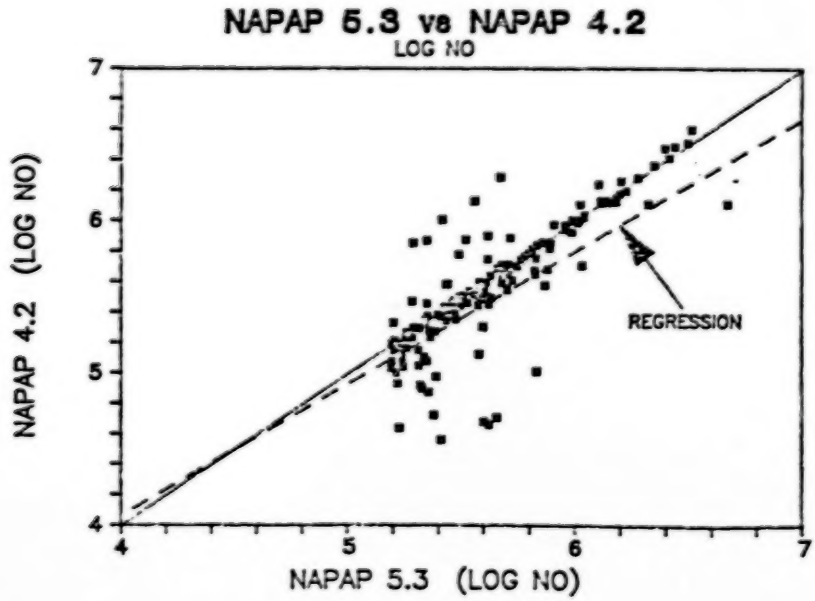


Figure 3. Comparison of NAPAP 5.3 and NAPAP 4.2 gridded NO emissions for the 200 strongest source cells in the Northeastern U.S. ROM domain.

emissions estimates do compare favorably with independent estimates made by Lamb, Westberg, et al. (1983b) for Pennsylvania. Preliminary model executions indicate that the addition of biogenic hydrocarbon emissions appears to improve model performance.

After final verification of the "raw" data, ROM processors are executed in a predetermined sequence. Because of the complex interrelationships among processors and the large number of files produced, the execution of the processors has been automated. A Formulation Management System (FOREMAN) automatically generates runstreams, allocates disk space and assigns input/output file names required for execution of all processors for a specified 3-day simulation period. FOREMAN, a computer resident program, then initiates job execution and checks status of all processor executions every half hour. When all required input files for a specific processor have been generated then that processor execution is automatically initiated.

The automation of this execution process provides an excellent means of producing a comprehensive audit trail - a listing confirming what actual input data sets and processor versions were used for a specific execution. It also minimizes the potential for human error. This is of critical concern when multiple research and policy model applications are being performed simultaneously. The data file audit information (file creation date, simulation date, date of last update, parameter names and units, etc.) is explicitly written on the header record of each file. Thus each data file is self-documenting and this header information is printed each time a file is accessed. The software audit trail is implemented by inserting in each major software component - program and/or subroutine - a unique entry point which prints the version identification of that component. Thus at the beginning of each processor execution all "special" entry points are called to print a summary of software identification. These techniques are enforced through the software certification process.

The output of each processor is carefully reviewed according to written verification procedures specific to each processor. These procedures document all quality control checks to be performed and potential sources of error if certain conditions are found to exist. Strict adherence to these procedures ensure consistent quality of the data. For completeness, every value calculated for each parameter is automatically compared with predefined minimum and maximum values for that parameter. Those values out of range are flagged for further review.

In many cases graphical analysis is performed on a parameter over the entire model domain to look for spatial inconsistencies. These fields are frequently compared with other gridded fields when a specific relationship between parameters exists. A comparison of gridded values in all 3 layers of the model is often performed to review the vertical structure of a given parameter. Preparation of the final B-Matrix input file is not initiated until all quality control procedures are verified as complete for a given 3-day simulation.

## Model Evaluation Approach

The next step in the model verification process is to establish quantitatively how close the model predictions are to pollutant concentration values measured under the simulated emissions and meteorological conditions. From a policy perspective, there is also a need to demonstrate that the model is capable of accurately simulating those phenomena of particular importance for regulatory support. Those phenomena differ

with each application but, at a minimum, include multiday transport of ozone across state and national boundaries, the magnitude of hourly ozone maxima which form the basis for the current U.S. National Ambient Air Quality Standards (NAAQS), and the spatial distribution of seasonally averaged ozone for use in health and welfare benefit assessments.

A detailed approach for ROM evaluation is described by Schere and Fabrick (1985). This approach consists of three levels of analysis. In the first level, ambient air quality measurements are analyzed to characterize important features of pollutant concentration on both temporal and spatial scales. This analysis considers ground and aircraft measurements with emphasis on surface ozone concentrations. Knowledge of the existence and extent of ozone plumes typically found downwind of large urban areas is critical for evaluating how well ROM predicts peak ozone on an episodic basis. An important question is whether or not the ozone plumes are wide enough to be resolved by the 18.5 km grid resolution of ROM. In addition, review of the NMHC/$NO_x$ ratio of air quality data in urban areas can provide an indication of the local potential for ozone formation.

The second level of analysis evaluates the capability of ROM to accurately predict hourly ozone concentrations and daily spatial and temporal patterns for a single realization of an episode. A realization refers to a specific wind field used to drive the transport in the model. Standard statistics --absolute deviation, variance, bias, variance of residuals, linear regression -- are computed for various combinations of observed versus predicted concentrations. ROM grid predictions are paired with associated monitoring station values as receptor class averages where grid cells are grouped by common characteristics, such as emissions density or distance from major population centers. Peak hourly predictions are analyzed separately to look for a systematic bias which ultimately might impact emission reduction criteria. Daily maximum values over all measurement sites in the downwind extent of an urban source plume are paired in several ways with model predictions, progressing from restrictive (same location) to unconstrained such as peak observed versus peak predicted regardless of location. The analysis also includes a comparison of the spatial pattern of predicted versus observed ozone as well as of residual concentration fields.

The third level of analysis evaluates the probability distribution of ROM predictions based on related families of wind fields. For this analysis ROM is applied using approximately 10 different wind fields for the same meteorological scenario. Each wind field is consistent with the observed meteorology for the scenario at all measurement sites and satisfies the physical laws governing atmospheric flow (see Lamb and Hati, 1987). Appropriate analysis of the resulting concentration distributions can provide quantitative estimates of the inherent uncertainty associated with the prediction of ozone on a regional scale. This type of information is very useful in the regulatory framework.

Preliminary Evaluation of First Generation ROM

The first generation ROM has been evaluated on a two-day episode in the Northeastern U.S. (Schere, 1986). The period August 3-4, 1979 was characterized by relatively high ozone concentrations in the southern Great Lakes area where clear skies persisted. Eastern seaboard cities which experienced clouds and showers in the vicinity of a stationary front recorded intermittent periods of relatively high ozone. The highest observed hour-average ozone monitored at a surface site during the period was 159 ppb. The study was designed to evaluate ROM's ability to predict hourly and maximum ozone concentrations. Results indicate a 6% average underprediction when all hours and surface monitoring sites are considered.

When observed and predicted pairs are restricted to ozone values greater than 50 ppb the average performance improved to a 1% underprediction. The maximum daily ozone values showed an 8% average underprediction for the restricted subset. An analysis of individual ozone plumes during the episode showed averge model performance for predicting the plume maximum concentration level to lie between 22% underprediction and 38% overprediction.

Preliminary efforts to evaluate the second generation ROM have just begun. Figure 4 compares maximum measured 1-hour averaged ozone concentrations during the period July 12-17, 1980 with predicted maximum 1-hour values during the same period. There appears to be a good correlation both in magnitude and location. Also a brief study was done to assess the impact of biogenic emissions on ROM ozone predictions. The addition of biogenic hydrocarbons increased estimated ozone from 20 - 60 ppb in the Appalachians and, in particular, downwind of large $NO_x$ plumes. In the previous first generation ROM evaluation these particular areas had shown consistent underprediction.

## ROM APPLICATIONS

Even though ROM is not yet fully evaluated there have been numerous requests for applications to provide some insight into the potential impact of various emission control strategies. Lamb (1986) has reported the results of one preliminary study with the first generation ROM. The purpose of this study was to evaluate the effects of urban control strategies on rural ozone concentration. ROM was executed for a 9-day period, 23 - 31 July 1980, with base year 1980 NAPAP 4.2 emissions and again with reduced emissions based on State Implementation Plan projected 1987 emission controls. On average VOC emissions were reduced by 32% and $NO_x$ emissions were reduced by 8%. ROM predicted ozone was grouped into four receptor cell categories: urban, suburban, rural, and wilderness. Overall, the analysis indicated that peak concentrations within each receptor class were reduced by larger percentages than the mean values and that emissions reductions caused a delay in ozone formation as well as reducing the total quantity produced.

An important quality control feature was incorporated in ROM to ensure that the effects seen in comparing model results are due to emission changes only and not spurious data errors in other model inputs. After all, a primary use of ROM is to assess the effect of emission changes on ozone formation. In each execution of ROM a dummy emissions species, a tracer, is emitted at a fixed rate from predetermined locations. This tracer species decays at a rate proportional to the local photolysis rate of $NO_2$ but has no other chemical interaction; thus it is dependent on meteorology alone. Therefore, for two model executions of the same meteorological scenario, as in the case described above, the predicted value of this dummy species must be exactly equivalent throughout space and time to serve as final proof that emission changes alone are the source of any difference in the resulting predictions.

The second generation ROM has been applied to assess the contribution of Treatment Storage Disposal Facility (TSDF) hydrocarbon emissions to regional ozone levels. Preliminary results indicate that TSDF emissions contribute very little to regional ozone, but uncertainties in the emissions data raise questions about the validity of that interpretation. The accuracy of emission inventories, in fact, is one of the most critical issues today regarding the use of ROM for regulatory support.

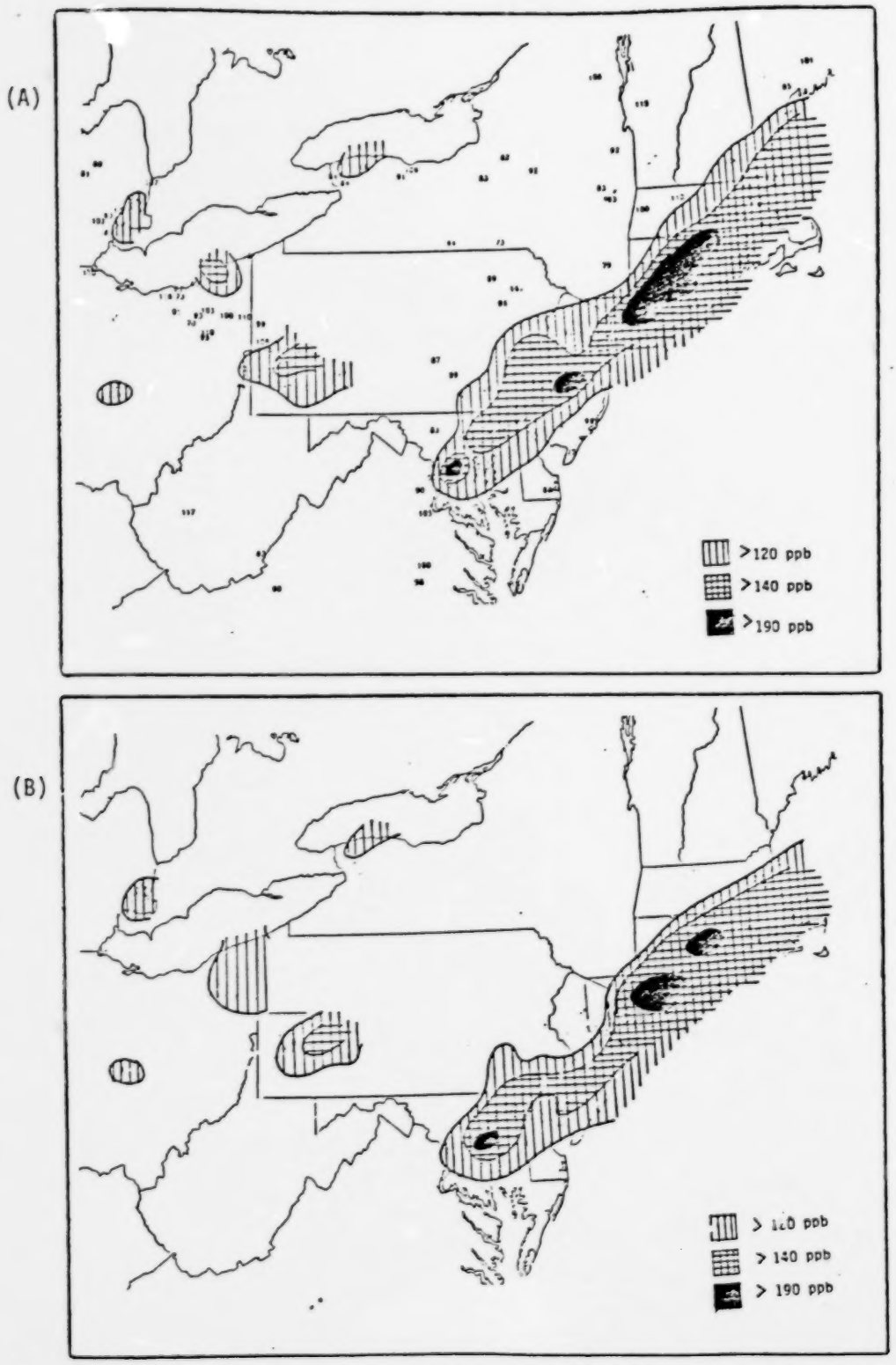


Figure 4. (A). Maximum measured 1-hour averaged ozone concentration at SAROAD sites during the period 12-17 July 1980;
(B). Same as (A) except model predictions replace measured values at SAROAD sites.

## CONCLUSIONS

This paper presents an overview of the verification procedures that are an essential part of the Regional Oxidant Modeling program. The major point of emphasis is that quality control procedures must be carefully integrated into every step of the development and application efforts. Verification and evaluation procedures should be designed to demonstrate the ability of the model to perform specifically for the intended applications. Preliminary studies have shown ROM to be an effective tool for control strategy evaluation. But a formal evaluation of ROM must be completed and uncertainties in the emissions inventories must, at minimum, be quantified before interpretation of model results can effectively support regulatory decision making.

## ACKNOWLEDGEMENTS

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